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STRUCTURE FILE UPDATES: 31 OCT 2005 HIGHEST RN 866452-21-3  
DICTIONARY FILE UPDATES: 31 OCT 2005 HIGHEST RN 866452-21-3

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\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
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=> fil hcap

FILE 'HCAPLUS' ENTERED AT 14:51:07 ON 01 NOV 2005  
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FILE COVERS 1907 - 1 Nov 2005 VOL 143 ISS 19

FILE LAST UPDATED: 31 Oct 2005 (20051031/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 14:12:59 ON 01 NOV 2005)

FILE 'HCAPLUS' ENTERED AT 14:13:09 ON 01 NOV 2005  
E US20040033910/PN

L1 1 S E3  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 14:14:04 ON 01 NOV 2005  
L2 8 S E1-8

FILE 'HCAPLUS' ENTERED AT 14:16:12 ON 01 NOV 2005  
L3 1 S L1 AND L2

FILE 'REGISTRY' ENTERED AT 14:23:16 ON 01 NOV 2005  
L4 1 S 653603-12-4/RN  
L5 STR 653603-12-4  
L6 0 S L5  
L7 STR L5  
L8 1 S L7  
L9 STR L7  
L10 2 S L9  
L11 19 S L9 FUL  
SAV L11 COSTALES097/A

FILE 'HCAPLUS' ENTERED AT 14:45:49 ON 01 NOV 2005  
L12 5 S L11

FILE 'STNGUIDE' ENTERED AT 14:48:03 ON 01 NOV 2005

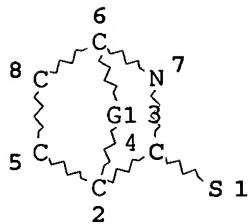
FILE 'HCAPLUS' ENTERED AT 14:48:44 ON 01 NOV 2005  
L13 1 S L1 AND L12

FILE 'STNGUIDE' ENTERED AT 14:48:59 ON 01 NOV 2005  
SET COST OFF

FILE 'REGISTRY' ENTERED AT 14:51:04 ON 01 NOV 2005

FILE 'HCAPLUS' ENTERED AT 14:51:07 ON 01 NOV 2005

=> d 112 que stat  
L9 STR



VAR G1=O/S/N/C

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 1

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L11 19 SEA FILE=REGISTRY SSS FUL L9

L12 5 SEA FILE=HCAPLUS L11

=&gt; d 112 bib abs hitstr ind 1-

YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/ (N) :y

L12 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:142784 HCAPLUS

DN 140:202191

TI Bicyclic thioamides as ashless, phosphorus-free and metal-free lubricating oil additives

IN Mukkamala, Ravindranath

PA USA

SO U.S. Pat. Appl. Publ., 5 pp.

CODEN: USXXCO

DT Patent

LA English

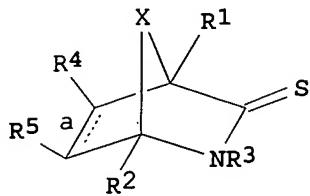
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004033910	A1	20040219	US 2003-636097	200308 07
	EP 1394240	A1	20040303	EP 2003-254694	200307 28
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2004162029 A2 20040610 JP 2003-287841 200308 06					

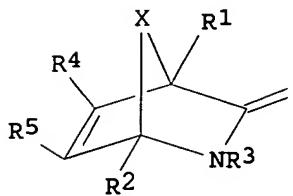
← Applicant

PRAI US 2002-401541P  
 OS MARPAT 140:202191  
 GI

P 20020807



I



II

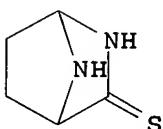
AB Non-metallic, phosphorus-free lubrication oil additives are of general structure I, in which X = -O-, -S-, -NR6-, or -CR7R8-; R1, R2, R4, R5, R7, and R8 are H, alkyl, alkenyl, aryl, or aralkyl, and; R3 and R6 are H, alkyl, alkenyl, aryl, aralkyl, alkanoyl, or aroyl. R3 is preferably C6-22-alkyl or -alkenyl, aryl, or aralkyl. Other addnl. compds. are of structure II (prepd. from I), in which R6 is B3, H, alkyl, alkenyl, aryl, aralkyl, alkanoyl, or aroyl; B1-3 are -CHR12-CHR13-CO2R14, -CR10R11-NHR9, -C(:O)NHR15, -C(:S)NHR15, or R16; R10, R11, and R14 are H, alkyl, alkenyl, aryl, or aralkyl; R16 is H or C1-4-alkyl; R9 and R15 are alkyl, alkenyl, aryl, or aralkyl. The additives, present at 0.1-20 wt.% in a lubricating oil, are substitutes for conventional zinc dialkyldithiophosphates.

IT 653603-12-4D, 2,7-Diazabicyclo[2.2.1]heptane-3-thione, derivs. 653603-13-5D, derivs. 653603-14-6D, derivs. 653603-15-7D, 2-Azabicyclo[2.2.1]heptane-3-thione, derivs. 653603-16-8D, derivs. 653603-17-9D, derivs. 653603-18-0D, derivs. 653603-19-1D, 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, derivs.

RL: MOA (Modifier or additive use); USES (Uses)  
 (additives; bicyclic thioamides as ashless, phosphorus-free and metal-free lubricating oil additives)

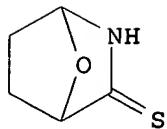
RN 653603-12-4 HCPLUS

CN 2,7-Diazabicyclo[2.2.1]heptane-3-thione (9CI) (CA INDEX NAME)

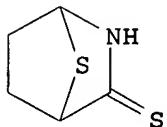


RN 653603-13-5 HCPLUS

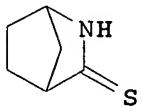
CN 7-Oxa-2-azabicyclo[2.2.1]heptane-3-thione (9CI) (CA INDEX NAME)



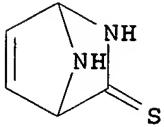
RN 653603-14-6 HCPLUS  
 CN 7-Thia-2-azabicyclo[2.2.1]heptane-3-thione (9CI) (CA INDEX NAME)



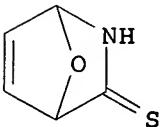
RN 653603-15-7 HCPLUS  
 CN 2-Azabicyclo[2.2.1]heptane-3-thione (9CI) (CA INDEX NAME)



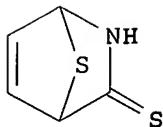
RN 653603-16-8 HCPLUS  
 CN 2,7-Diazabicyclo[2.2.1]hept-5-ene-3-thione (9CI) (CA INDEX NAME)



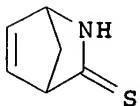
RN 653603-17-9 HCPLUS  
 CN 7-Oxa-2-azabicyclo[2.2.1]hept-5-ene-3-thione (9CI) (CA INDEX NAME)



RN 653603-18-0 HCPLUS  
 CN 7-Thia-2-azabicyclo[2.2.1]hept-5-ene-3-thione (9CI) (CA INDEX NAME)



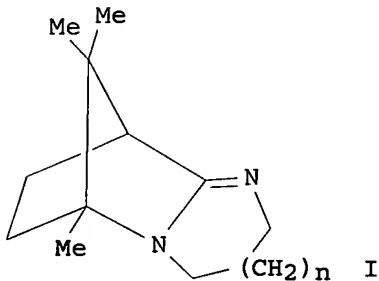
RN 653603-19-1 HCPLUS  
 CN 2-Azabicyclo[2.2.1]hept-5-ene-3-thione (9CI) (CA INDEX NAME)



IC ICM C10M135-32  
 INCL 508221000; 508261000; 508242000; 546112000; 546114000; 546116000  
 CC 51-8 (Fossil Fuels, Derivatives, and Related Products)  
 Section cross-reference(s): 24, 28  
 ST bicyclic thioamide lubricating oil additive; antiwear ashless  
 lubricating oil additive bicyclic thioamide; zinc dithiophosphate  
 substitute bicyclic thioamide lubricant additive  
 IT Lubricating oil additives  
 (antiwear; bicyclic thioamides as ashless, phosphorus-free and  
 metal-free lubricating oil additives)  
 IT Heterocyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (bicyclic, nitrogen, additives; bicyclic thioamides as ashless,  
 phosphorus-free and metal-free lubricating oil additives)  
 IT Heterocyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (bicyclic, oxygen, additives; bicyclic thioamides as ashless,  
 phosphorus-free and metal-free lubricating oil additives)  
 IT Heterocyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (bicyclic, sulfur, additives; bicyclic thioamides as ashless,  
 phosphorus-free and metal-free lubricating oil additives)  
 IT Thioamides  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (bicyclic; bicyclic thioamides as ashless, phosphorus-free and  
 metal-free lubricating oil additives)  
 IT Bicyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (heterocyclic, nitrogen, additives; bicyclic thioamides as  
 ashless, phosphorus-free and metal-free lubricating oil  
 additives)  
 IT Bicyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (heterocyclic, oxygen, additives; bicyclic thioamides as ashless,  
 phosphorus-free and metal-free lubricating oil additives)  
 IT Bicyclic compounds  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (heterocyclic, sulfur, additives; bicyclic thioamides as ashless,

phosphorus-free and metal-free lubricating oil additives)  
 IT Lubricating oil additives  
 (multifunctional; bicyclic thioamides as ashless, phosphorus-free  
 and metal-free lubricating oil additives)  
 IT 653603-12-4D, 2,7-Diazabicyclo[2.2.1]heptane-3-thione,  
 derivs. 653603-13-5D, derivs. 653603-14-6D,  
 derivs. 653603-15-7D, 2-Azabicyclo[2.2.1]heptane-3-thione,  
 derivs. 653603-16-8D, derivs. 653603-17-9D,  
 derivs. 653603-18-0D, derivs. 653603-19-1D,  
 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, derivs.  
 RL: MOA (Modifier or additive use); USES (Uses)  
 (additives; bicyclic thioamides as ashless, phosphorus-free and  
 metal-free lubricating oil additives)

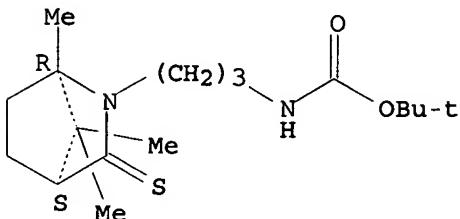
L12 ANSWER 2 OF 5 HCPLUS COPYRIGHT 2005 ACS on STN  
 AN 2000:799014 HCPLUS  
 DN 134:115933  
 TI A novel synthesis of chiral DBU/DBN-related molecules for use in  
 asymmetric base catalysis  
 AU Kotsuki, Hiroyoshi; Sugino, Atsushi; Sakai, Hiromitsu; Yasuoka,  
 Hiroko  
 CS Laboratory of Natural Products Synthesis, Faculty of Science, Kochi  
 University, Kochi, 780-8520, Japan  
 SO Heterocycles (2000), 53(11), 2561-2567  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PB Japan Institute of Heterocyclic Chemistry  
 DT Journal  
 LA English  
 OS CASREACT 134:115933  
 GI



AB The sterically hindered chiral DBU/DBN-related mols. I [n = 1, 2]  
 were prep'd. from (+)-camphor lactam. The value of I as chiral org.  
 base catalysts is exemplified by their use in asym. Michael addn.  
 reactions of Me 1-oxo-2-indancarboxylate with MeCOCH:CH2.  
 IT 320573-80-6P 320573-81-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. of chiral diazatricycloalkenes as catalysts for asym.  
 Michael addns.)  
 RN 320573-80-6 HCPLUS  
 CN Carbamic acid, [3-[(1R,4S)-1,7,7-trimethyl-3-thioxo-2-

azabicyclo[2.2.1]hept-2-yl]propyl-, 1,1-dimethylethyl ester (9CI)  
(CA INDEX NAME)

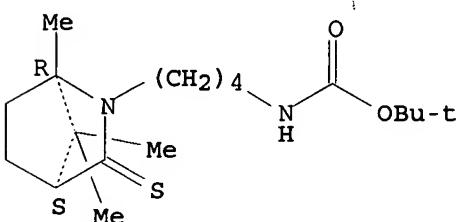
Absolute stereochemistry.



RN 320573-81-7 HCPLUS

CN Carbamic acid, [4-[(1R,4S)-1,7,7-trimethyl-3-thioxo-2-azabicyclo[2.2.1]hept-2-yl]butyl]-, 1,1-dimethylethyl ester (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))

ST diazatricycloalkene prepn chiral catalyst stereoselective Michael addn

IT Michael reaction

Michael reaction catalysts

(stereoselective; prepn. of chiral diazatricycloalkenes as catalysts for asym. Michael addns.)

IT 320573-82-8P 320573-83-9P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of chiral diazatricycloalkenes as catalysts for asym. Michael addns.)

IT 78-94-4, Methyl vinyl ketone, reactions 2162-33-6 22955-77-7  
24326-89-4 51326-51-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of chiral diazatricycloalkenes as catalysts for asym. Michael addns.)

IT 105064-28-6P 320573-75-9P 320573-76-0P 320573-77-1P

320573-78-2P 320573-79-3P 320573-80-6P

**320573-81-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of chiral diazatricycloalkenes as catalysts for asym. Michael addns.)

IT 66152-63-4P 79298-08-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of chiral diazatricycloalkenes as catalysts for asym.  
Michael addns.)RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:570954 HCAPLUS

DN 131:286165

TI Conformational properties and chiroptical spectra of lactams and  
thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and  
3-azabicyclo[3.2.1]octane skeletonsAU Polonski, Tadeusz; Milewska, Maria J.; Konitz, Antoni; Gdaniec,  
Maria

CS Department of Chemistry, Technical University, Gdansk, 80-952, Pol.

SO Tetrahedron: Asymmetry (1999), 10(13), 2591-2604

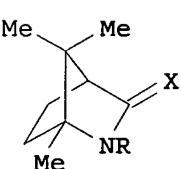
CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier Science Ltd.

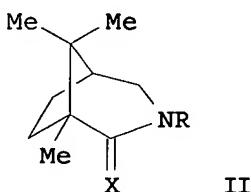
DT Journal

LA English

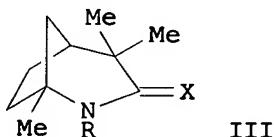
GI



I



II



III

AB The CD spectra of several bicyclic lactams and thiolactams were measured in different solvents. The concn. dependence of the spectra obsd. in hydrocarbon solvents was attributed to shifts in the equil. between monomer and hydrogen-bonded dimer forms. The CD of some compds. is characterized by unusually strong Cotton effects resulting from non-planarity of the amide bonds due to internal strain of the bicyclic skeletons. The X-ray crystallog. structures of I(R,X given: H<sub>2</sub>O;H,S), II(R,X given: Me<sub>2</sub>O;Me,S) and III(R,X given: H<sub>2</sub>O;Me,O) showed different degrees of distortion of the amide or thioamide moieties from planarity, which causes inherent chirality of the chromophores and profoundly affects the Cotton effect sign and magnitude. This distortion also restricts application of the sector rules for prediction of the n-π\* CD

sign, since they can be used only for compds. with planar chromophores.

IT 246044-07-5P 246044-09-7P 246044-11-1P

246044-12-2P

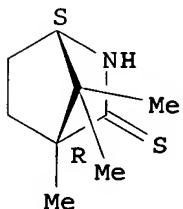
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(conformational properties and chiroptical spectra of lactams and thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and 3-azabicyclo[3.2.1]octane skeletons)

RN 246044-07-5 HCPLUS

CN 2-Azabicyclo[2.2.1]heptane-3-thione, 4,7,7-trimethyl-, (1S,4R)- (9CI) (CA INDEX NAME)

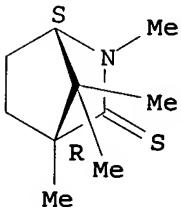
Absolute stereochemistry. Rotation (-).



RN 246044-09-7 HCPLUS

CN 2-Azabicyclo[2.2.1]heptane-3-thione, 2,4,7,7-tetramethyl-, (1S,4R)- (9CI) (CA INDEX NAME)

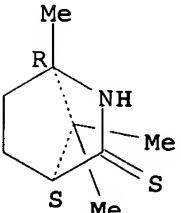
Absolute stereochemistry. Rotation (-).



RN 246044-11-1 HCPLUS

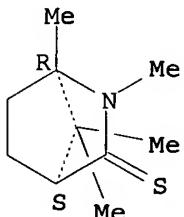
CN 2-Azabicyclo[2.2.1]heptane-3-thione, 1,7,7-trimethyl-, (1R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 246044-12-2 HCAPLUS  
 CN 2-Azabicyclo[2.2.1]heptane-3-thione, 1,2,7,7-tetramethyl-, (1R,4S)-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



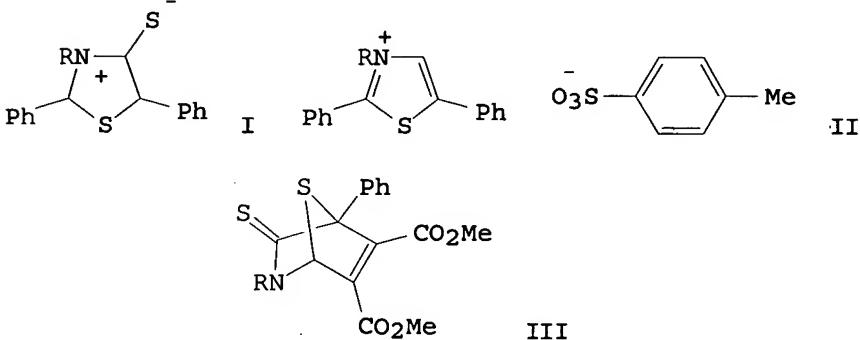
CC 22-11 (Physical Organic Chemistry)  
 Section cross-reference(s): 75  
 ST CD spectra bicyclic lactam thiolactam; crystallog bicyclic lactam  
 thiolactam; conformation bicyclic lactam thiolactam  
 IT Circular dichroism  
 Conformation  
 Cotton effect  
 Crystal structure  
 Molecular structure  
 Strain energy  
 UV and visible spectra  
 (conformational properties and chiroptical spectra of lactams and  
 thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and  
 3-azabicyclo[3.2.1]octane skeletons)  
 IT Bicyclic compounds  
 Lactams  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (conformational properties and chiroptical spectra of lactams and  
 thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and  
 3-azabicyclo[3.2.1]octane skeletons)  
 IT Dimers  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (hydrogen-bonded; conformational properties and chiroptical  
 spectra of lactams and thiolactams with 2-  
 azabicyclo[2.2.1]heptane, 2- and 3-azabicyclo[3.2.1]octane  
 skeletons)  
 IT Lactams  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (thio-; conformational properties and chiroptical spectra of  
 lactams and thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and  
 3-azabicyclo[3.2.1]octane skeletons)  
 IT 24326-88-3P 24326-89-4P 107073-56-3P 107073-62-1P  
 107133-28-8P 246044-06-4P 246044-07-5P  
 246044-09-7P 246044-10-0P 246044-11-1P  
 246044-12-2P 246044-17-7P 246044-18-8P 246044-19-9P  
 246044-20-2P 246044-21-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(conformational properties and chiroptical spectra of lactams and thiolactams with 2-azabicyclo[2.2.1]heptane, 2- and 3-azabicyclo[3.2.1]octane skeletons)

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN  
AN 1985:184997 HCAPLUS  
DN 102:184997  
TI Studies on mesoionic compounds. XIV. Synthesis of mesoionic 1,3-thiazolium-4-thiolates  
AU Takezawa, Katsushi; Nomura, Keiichi; Yoshii, Eiichi; Masuda, Katsutada  
CS Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930, Japan  
SO Chemical & Pharmaceutical Bulletin (1984), 32(11), 4637-40  
CODEN: CPBTAL; ISSN: 0009-2363  
DT Journal  
LA English  
OS CASREACT 102:184997  
GI

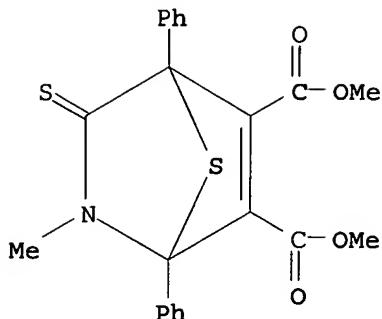


AB 3-Alkyl-2,5-diphenyl-1,3-thiazolium-4-thiolate I (R = Me, Et, CH<sub>2</sub>Ph) were prep'd. by exchange of the exocyclic O of the mesoionic 4-olate with S via O-methylation or by base-catalyzed thiation of the N-alkyl-1,3-thiazolium compd II. I underwent cycloaddn. with MeO<sub>2</sub>CC.tplbond.CCO<sub>2</sub>Me to give thermally stable bicyclic compds. III.

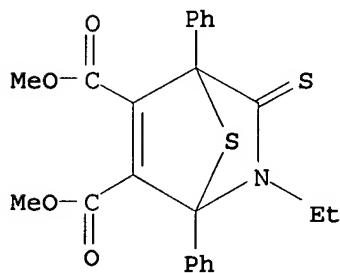
IT 96207-20-4P 96207-21-5P 96207-22-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 96207-20-4 HCAPLUS

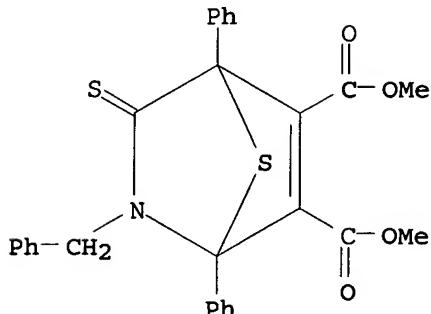
CN 7-Thia-2-azabicyclo[2.2.1]hept-5-ene-5,6-dicarboxylic acid, 2-methyl-1,4-diphenyl-3-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 96207-21-5 HCAPLUS

CN 7-Thia-2-azabicyclo[2.2.1]hept-5-ene-5,6-dicarboxylic acid,  
2-ethyl-1,4-diphenyl-3-thioxo-, dimethyl ester (9CI) (CA INDEX  
NAME)

RN 96207-22-6 HCAPLUS

CN 7-Thia-2-azabicyclo[2.2.1]hept-5-ene-5,6-dicarboxylic acid,  
1,4-diphenyl-2-(phenylmethyl)-3-thioxo-, dimethyl ester (9CI) (CA  
INDEX NAME)

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

ST thiazoliumthiolate prepn cycloaddn acetylenedicarboxylate;  
thiaazabicycloheptenethone; mesoionic thiazoliumthiolate

IT Meso-ionic compounds

RL: SPN (Synthetic preparation); PREP (Preparation)

(thiazolium thiolates, prepn. and cycloaddn. of, with acetylenedicarboxylate)

IT 96207-11-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and methylation of)

IT 96207-17-9P 96207-18-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and reaction of, with acetylenedicarboxylate)

IT 56922-47-5P 96207-16-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and reaction of, with sulfur)

IT 96207-12-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and reaction of, with trimethyloxonium tetrafluoroborate)

IT 96207-14-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (prepn. and thiolation of)

IT 96207-19-1P 96207-20-4P 96207-21-5P  
 96207-22-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

IT 80-48-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with 2,5-diphenylthiazole)

IT 3704-40-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with alkyl p-toluenesulfonates)

IT 762-42-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with alkylidiphenylthiazolium thiolates)

IT 5310-14-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with bromophenylacetic acid)

IT 80-40-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with diphenylthiazole)

IT 4870-65-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with methylthiobenzamide)

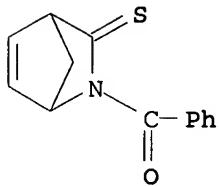
L12 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN  
 AN 1966:420707 HCAPLUS  
 DN 65:20707  
 OREF 65:3826e-f  
 TI Diels-Alder synthesis with acetyl and benzoyl isothiocyanates  
 AU Arbuzov, B. A.; Zobova, N. N.  
 CS State Univ., Kazan  
 SO Doklady Akademii Nauk SSSR (1966), 167(4), 815-18  
 CODEN: DANKAS; ISSN: 0002-3264  
 DT Journal  
 LA Russian

AB Keeping benzoyl isothiocyanate with 1 mole butadiene in a sealed tube 6-7 months gave after treatment with dry Et<sub>2</sub>O 45.3% N-benzoyl-2-thiono-1,2,3,6-tetrahydropyridine, m. 97-8°; acetyl isothiocyanate gave the N-acetyl analog, 40.7%, m. 78-80°. Reaction with isoprene performed in the presence of hydroquinone gave, resp., 44.5% 4(or 5)-methyl-N-benzoyl-2-thiono-1,2,3,6-tetrahydropyridine, m. 99-101°, and 39.2% 4(or 5)-methyl-N-acetyl-2-thiono-1,2,3,6-tetrahydropyridine, m. 82-3°. Similar reaction with 2,3-dimethyl-1,3-butadiene gave 46% 4,5-dimethyl-N-benzoyl-2-thiono-1,2,3,6-tetrahydropyridine, m. 146°, and 42.5% 4,5-dimethyl-N-acetyl-2-thiono-1,2,3,6-tetrahydropyridine, m. 93.5-5°. Cyclopentadiene gave 50.6% N-benzoyl-3-thiono-2-azabicyclo[2.2.1]-5-heptene, m. 125.5-26°, and 49.8% N-acetyl analog, m. 91-2°. Ir spectra are reported.

IT 6431-29-4, 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, 2-benzoyl- 6431-30-7, 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, 2-acetyl- (prepn. and spectrum of)

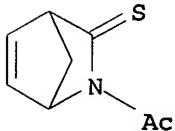
RN 6431-29-4 HCPLUS

CN 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, 2-benzoyl- (7CI, 8CI) (CA INDEX NAME)



RN 6431-30-7 HCPLUS

CN 2-Azabicyclo[2.2.1]hept-5-ene-3-thione, 2-acetyl- (7CI, 8CI) (CA INDEX NAME)



CC 37 (Heterocyclic Compounds (One Hetero Atom))

IT Spectra, infrared  
(of Diels-Alder adducts with acetyl and benzoyl isothiocyanates)

IT Diels-Alder reaction  
(of acetic acid anhydride with isothiocyanic acid or benzoic acid anhydride with isothiocyanic acid)

IT Acetic acid, anhydride with isothiocyanic acid  
(Diels-Alder reaction with)

IT 532-55-8, Benzoic acid, anhydride with isothiocyanic acid  
(Diels-Alder reaction with)

IT 6431-24-9, 2(1H)-Pyridinethione, 1-benzoyl-3,6-dihydro- 6431-25-0,

2(1H)-Pyridinethione, 1-acetyl-3,6-dihydro- 6431-26-1,  
2(1H)-Pyridinethione, 1-benzoyl-3,6-dihydro-4-methyl- (?)  
6431-27-2, 2(1H)-Pyridinethione, 1-benzoyl-3,6-dihydro-4,5-dimethyl-  
6431-28-3, 2(1H)-Pyridinethione, 1-acetyl-3,6-dihydro-4,5-dimethyl-  
6431-29-4, 2-Azabicyclo[2.2.1]hept-5-ene-3-thione,  
2-benzoyl- 6431-30-7, 2-Azabicyclo[2.2.1]hept-5-ene-3-  
thione, 2-acetyl- 6545-84-2, 2(1H)-Pyridinethione,  
1-acetyl-3,6-dihydro-4-methyl- (?) 13250-44-7, 2(1H)-  
Pyridinethione, 1-benzoyl-3,6-dihydro-5-methyl- (?) 13250-45-8,  
2(1H)-Pyridinethione, 1-acetyl-3,6-dihydro-5-methyl- (?)  
(prepn. and spectrum of)

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